# SPA+RPA approach to canonical and grandcanonical treatments of nuclear level densities

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## Abstract

Using an exactly solvable pairing model Hamiltonian in the static path approximation together with small-amplitude quantal fluctuation corrections in random phase approximation (SPA+RPA), we have analyzed the behaviour of canonical (number projected) and grandcanonical treatments of nuclear level densities as a function of temperature and number of particles. For small particle numbers at a low temperature, we find that though the grandcanonical partition function in SPA+RPA approach is quite close to its exact value, the small errors in its estimation causes significant suppression of level density obtained using number projected partition function. The results are also compared with the smoothed out exact values of level density. Within this model study, it appears that due to saddle point approximation to multiple Laplace-back transform, the grandcanonical treatment of level density at low temperature may be reliable only for relatively large number of particles.

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The familiar Bethe formula[1, 2] for the level density, because of its simplicity, has been widely used to perform the statistical analysis of nuclear reactions. This level density formula takes a simple form due to (i) the connection of grandcanonical partition function with microcanonical partition function (level density) by a saddle point approximation in the evaluation of the traces over the states[3] and (ii) the grandcanonical partition function itself is approximated using independent single particle spectrum which is further assumed to be equidistant. Recently, a more realistic value of the level density[4]-[6] in saddle point approximation is obtained using a grandcanonical partition function in static path approximation[7, 8] which accounts for the large-amplitude thermal fluctuations. The method of saddle point approximation can be generalized in order to treat the level densities that are characterized by a set of quantum numbers, provided, these quantum numbers are composed additively of contributions from the single particle states (e.g. excitation energy $(E^*)$, number of protons $(N_p)$ or neutrons $(N_n)$, angular momentum, parity etc.). For instance, consider the system consisting of one kind of particles(protons or neutrons). The exact level density,

$$\rho(E, N) = \sum_{\lambda} \delta(E - E_{\lambda})\delta(N - N_{\lambda}) \tag{1}$$

can also be obtained by double Laplace-back transform of the grandcanonical partition function $\mathcal{Z}(\beta, \alpha)$ as

$$\rho(E, N) = (\frac{1}{2\pi i})^2 \int \int_{-i\infty}^{+i\infty} \mathcal{Z}(\beta, \alpha)e^{\beta E - \alpha N} d\beta d\alpha \tag{2}$$

In saddle point approximation, the level density $\hat{\rho}$ can be obtained directly in terms of canonical and grandcanonical partition functions as

$$\hat{\rho}^c = \frac{Z_N(\beta)e^{\beta E}}{\sqrt{2\pi} \left[\frac{\partial^2 ln \mathcal{Z}_N}{\partial \beta^2}\right]^{1/2}} \tag{3}$$

2

and

$$\hat{\rho}^g = \frac{\mathcal{Z}(\beta, \alpha)e^{\beta E - \alpha N}}{2\pi \left[\frac{\partial^2 ln\mathcal{Z}}{\partial \beta^2}\frac{\partial^2 ln\mathcal{Z}}{\partial \alpha^2} - \left(\frac{\partial^2 ln\mathcal{Z}}{\partial \alpha \partial \beta}\right)^2\right]^{1/2}}, \tag{4}$$

respectivley. The canonical partition function $Z_N(\beta)$ is given as

$$Z_N(\beta) = \frac{1}{2\pi i}\int_{-i\infty}^{+i\infty} Z(\beta, \alpha)e^{-\alpha N}d\alpha \tag{5}$$

In above equations, $\beta$ corresponds to inverse temperature $(1/T)$ and $\alpha = \mu\beta$ with $\mu$ being the chemical potential. Values of $\beta$ and $\alpha$ in eqs. (3) and (4) are chosen such that the saddle point conditions are satisfied, i.e.,

$$\frac{\partial ln\mathcal{Z}}{\partial \beta} + E = \frac{\partial ln\mathcal{Z}}{\partial \alpha} - N = 0. \tag{6}$$

From eqs. (3) and (4), it is clear that in general the canonical and grandcanonical treatments of level density would differ by the saddle point approximation to a single and a multiple Laplace-back transform of corresponding partition functions. A typical example, the grandcanonical treatment of level density for a given nucleus (i.e. fixed $N_p$ and $N_n$) as a function of excitation energy and angular momentum would require saddle point approximation to four Laplace-back transform[6, 9]. However, it has been pointed out in ref.[10] that the Bethe's formula for level density due to the saddle point approximation to several Laplace-back transform leads to a severe problem − violation of "microcanonical analyticity constraint" leading to a *measurable* differences between the microcanonical and grandcanonical treatments. Also, it can be seen in ref.[9, 11, 12] that at very high excitation energy the assumption of equidistant single particle spectrum in Bethe's formula gives rise to exponential deviations relative to more realistic values.

In this letter, we analyze the behaviour of the canonical and grandcanonical treatments of the level densities. For this purpose, we have used a recently developed method of exact functional representation[13, 14] to construct grandcanonical partition function for the interacting systems. It is clear from refs.[13, 15] that

the exact functional representation can be made easily numerically tractable using SPA+RPA (static path approximation+random phase approximation) approach. Moreover, it is shown in refs. [15, 16, 17] that when SPA+RPA approach applied to the grandcanonical partition function for the exactly solvable pairing and Lipkin model Hamiltonians, the results for $E^*$, $\hat{\rho}$ and heat capacity found to be very close to ones obtained using exact grandcanonical partition function. This approach has been applied to a realistic Hamiltonian also[18]. In what follows, we describe briefly, the SPA+RPA approach to canonical (number projected) and grandcanonical partition functions for exactly solvable pairing model.

We consider here the pairing Hamiltonian defined as

$$\hat{H} = -G\hat{P}^\dagger \hat{P} \tag{7}$$

where $G$ is the interaction strength, $\hat{P} = \sum_{k>0} \hat{a}_{\bar{k}} \hat{a}_k$. The index $k = 1, 2, ...\Omega$ with $\bar{k} = -k$ labels $2\Omega$ degenerate single particle states. Equation (7) can be rewritten in terms of quasi-spin operators as

$$\hat{H} = -G(\hat{J}^2 - \hat{J}_z^2 + \hat{J}_z) \tag{8}$$

where, $\hat{J}_x = \frac{1}{2}(\hat{P} + \hat{P}^\dagger)$, $J_y = \frac{i}{2}(\hat{P} - \hat{P}^\dagger)$ and $\hat{J}_z = \frac{1}{2}(\hat{N} - \Omega)$. Since, $\left[\hat{H}, \hat{J}^2\right] = \left[\hat{H}, \hat{J}_z\right] = 0$, the eigenvalues can be given as

$$E(J, M) = -G(J(J+1) - M^2 + M) \tag{9}$$

where,

$$M = \frac{1}{2}(N - \Omega) \tag{10}$$

with $N$ being the number of particles. The degeneracy factor for a given $J$ state is

$$g_J = \begin{pmatrix} 2\Omega \\ \Omega - 2J \end{pmatrix} - \begin{pmatrix} 2\Omega \\ \Omega - 2J - 2 \end{pmatrix}. \tag{11}$$

4

With these ingredients (eqs. 9-11), the exact level density can be obtained using eq. (1) as

$$\rho(E, N) = \sum_J g_J \delta(E - E(J)). \tag{12}$$

Here we have suppressed the $M$ dependence of eigenvalues (see eq.(9)) since it is fixed for a given number of particles. We define now a smooth version as

$$\bar{\rho}(E, N) = \sum_J g_J \Delta(E - E(J)) \tag{13}$$

which describes the exact average level density. We adopt a simple form for the spreading function $\Delta(x)$ as given below,

$$\Delta^n(x) = \frac{n}{\sqrt{\pi}} e^{-n^2 x^2} \tag{14}$$

where the parameter $n$ controls the width of spreading function. The above choice of $\Delta$-function essentially represents the dominant part of $\Delta = L_3^{1/2} e^{-x^2}$ as used in ref. [19].

It follows immediately from eqs. (3)-(5) that the level density in saddle point approximation can easily be obtained once the partition function is known. The exact canonical or grandcanonical partition function can be constructed as

$$\mathcal{Z}_N(\beta) = \sum_J g_J e^{-\beta E_J} \tag{15}$$

and

$$\mathcal{Z}(\beta, \alpha) = \sum_N e^{\alpha N} \sum_J g_J e^{-\beta E_J} \tag{16}$$

where $J = |M|, |M| + 1, ..., \Omega/2$ or $(\Omega - 1)/2$ depending on whether the $N$ is even or odd. It is worth mentioning here that eq. (15) can precisely be obtained by substituting eq. (16) in eq. (5) and using "Wick rotation" (i.e., $\alpha \to i\alpha$).

In SPA+RPA approach, $\mathcal{Z}(\beta, \alpha)$ takes the following form,

$$\tilde{\mathcal{Z}}(\beta, \alpha) = \frac{2\beta}{G} \int_0^\infty \Delta d\Delta e^{-\frac{\beta}{G}\Delta^2 + \alpha\Omega + \Omega S + 2\Omega ln[1+e^{-S}]} \mathcal{C}(\Delta) \tag{17}$$

where, the factor $\mathcal{C}(\Delta)$ as given below

$$\mathcal{C}(\Delta) = \prod_{m>0} \left[ \left[ 1 - \frac{\beta}{2}G\Omega\frac{Q^2}{S}\frac{tan\frac{S}{2}}{S^2+(\pi m)^2} \right] \left[ 1 - \frac{\beta}{2}G\Omega S\frac{tan\frac{S}{2}}{S^2+(\pi m)^2} \right] \right.$$
$$\left. + \left[ \frac{\beta}{2}G\Omega\frac{Q}{S}\frac{(\pi m)tan\frac{S}{2}}{S^2+(\pi m)^2} \right]^2 \right]^{-1} \quad (18)$$

is due to RPA, which accounts for small-amplitude quantal fluctuation corrections and $Q = \alpha + \frac{\beta}{2}G$, $S = \sqrt{Q^2 + \beta^2\Delta^2}$. With $\mathcal{C} = 1$, eq. (17) reduces to the partition function in SPA approach. The superscript tilde on $\mathcal{Z}$ in above equation is used to distinguish it from exact one.

The canonical (number projected) partition function can be obtained as follows

$$\tilde{\mathcal{Z}}_N(\beta) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\alpha\, e^{-i\alpha N} \tilde{\mathcal{Z}}(\beta, i\alpha) \quad (19)$$

where $\tilde{\mathcal{Z}}(\beta, i\alpha)$ is obtained using eq. (17) with $\alpha \to i\alpha$. The symmetric interval in $\alpha$ ensures that the partition function $\mathcal{Z}_N(\beta)$ will be real even if the approximate form for grand partition function is used.

We analyze now the saddle point approximation to the level density $\hat{\rho}$, evaluated using (a) SPA+RPA to canonical (number projected), (b) SPA+RPA to grandcanonical, (c) exact canonical and (d) exact grandcanonical partition functions. For the sake of comparison of these results with the smoothed out exact value of level density (eq. 13), we have plotted in figures 1 and 2 the ratio $\hat{\rho}/\bar{\rho}$ as a function of temperature for N $= 5$ and 10, respectively. To facilitate the further discussions, we denote $\hat{\rho}$ for the cases (a), (b), (c) and (d) by $\hat{\rho}^c_{rpa}$, $\hat{\rho}^g_{rpa}$, $\hat{\rho}^c_{ex}$ and $\hat{\rho}^g_{ex}$, respectively.

It can be seen from figures 1 and 2 that for all the cases, $\hat{\rho}/\bar{\rho}$ is quite different from unity at low temperature ($T \approx 0.25$ MeV) but with increase in temperature it approaches unity. The negative slope in $\hat{\rho}/\bar{\rho}$ vs $T$ curves indicates that the saddle point approximation is not applicable at very low temperature ($T <0.25$

6

MeV). So, we restrict ourselves to $T \geq 0.25$ MeV. Practically, for $N = 10$, the difference between $\hat{\rho}_{rpa}^{g}/\bar{\rho}$ and $\hat{\rho}_{ex}^{g}/\bar{\rho}$ is insignificant. On the other hand, for $N=5$ the difference between $\hat{\rho}_{rpa}^{c}/\bar{\rho}$ and $\hat{\rho}_{ex}^{c}/\bar{\rho}$ is noticeable at low $T$, whereas, this difference is small for $N=10$. It implies that, though the grandcanonical partition function in SPA+RPA approach becomes almost exact, the small errors in its estimation causes a significant suppression of the level density obtained using number projected partition function (eq. 19) at low $T$. Similar behaviour has been observed by Walt and Quick [17] for the heat capacity. In other words, at low temperature, the small errors in grandcanonical partition function enhances the difference between $\tilde{\mathcal{Z}}_{N}(\beta)$ and $\mathcal{Z}_{N}(\beta)$.

Let us now analyze the difference between canonical and grandcanonical treatments of level density and their deviations from the exact values. As discussed above (eqs. 3 and 4), in the present considerations, these treatments would differ only by the saddle point approximation to a single and a double Laplace-back transform. It is obvious from figures 1 and 2, the relative difference between the curves (a) and (b) or (c) and (d) at a fixed $T$ and $N$ is proportional to $\hat{\rho}^{c} - \hat{\rho}^{g}$. The difference between the level densities using canonical and grandcanonical treatments decreases with increase in temperature or number of particles. For instance at T = 0.35 MeV, the ratio $\hat{\rho}_{ex}^{c}/\hat{\rho}_{ex}^{g} = 20.83$ and 0.94 for N = 5 and 10, respectively, whereas, for T > 0.45 MeV this ratio becomes nearly equal to one. Finally, coming to the comparison between $\hat{\rho}$ and $\bar{\rho}$, we find that $\hat{\rho}/\bar{\rho}$ tends to unity with increase in number of particle and temperature. Thus, we can say that the saddle point approximation becomes almost exact with increase in temperature and particle numbers.

In conclusion, we have analyzed the canonical and grandcanonical treatments of the nuclear level densities in SPA+RPA approach which accounts for large-amplitude thermal fluctuations and small-amplitude quantal fluctuations. The re-

sults are compared with the corresponding exact ones. It is found that at low temperature the small errors in estimating the grandcanonical partition function cause significant suppression of level density obtained using number projected (canonical) partition function for small particle numbers. Also, we found that due to saddle point approximation to multiple Laplace-back transform, the grandcanonical treatment of the level density would be reliable at low temperature provided the particle number is relatively large. Furthermore, we must say that except at low temperatures where saddle point approximation itself is not reliable, a realistic value of level density can be obtained using SPA+RPA representation for the grandcanonical partition function.

## Acknowledgement

## Figure Captions

Figure 1: Plot for $\hat{\rho}/\bar{\rho}$ vs temperature for $N = 5$, where $\bar{\rho}$ represents the smoothed out exact (microcanonical) value of the level density and $\hat{\rho}$ correspond to the level density in a saddle point approximation which is obtained using (a) SPA+RPA approach to the canonical, (b) SPA+RPA approach to the grandcanonical, (c) exact canonical and (d) exact grandcanonical partition functions.

Figure 2: Same as figure 1 but for N = 10. Note that the curves (a) and (b) or (c) and (d) are very close to each other at all temperatures.

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